

Thermodynamic transition associated with irregularly ordered ground states in a lattice gas model

Shin-ichi Sasa §

Department of Pure and Applied Sciences, University of Tokyo, Komaba, Tokyo
153-8902, Japan

Abstract. A two-dimensional lattice gas model is proposed. The ground state of this model with a fixed density is neither periodic nor quasi-periodic. It also depends on system size in an irregular manner. On the other hand, it is ordered in the sense that the entropy density is zero in the thermodynamic limit. The existence of a thermodynamic transition associated with such irregularly ordered ground states is conjectured from a duality relation for a thermodynamic function. This conjecture is supported by a phenomenological argument and numerical experiments.

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1. Introduction

The ground state of a crystal is described by the repetition of a unit cell. Recalling that the repetition is a simple deterministic rule generating an infinite size pattern from a finite size pattern, we become curious about equilibrium systems with ground states described by other deterministic rules than the repetition. Note that the entropy density of such deterministic ground states is zero in the thermodynamic limit. In this sense, the ground states are ordered as observed in crystals. We call them *irregularly ordered ground states*. In this paper, we are concerned with thermodynamic transitions associated with irregularly ordered ground states.

We shall give a precise definition of irregularly ordered ground states by considering some examples. First, quasi-crystals provide aperiodic ground states [1]. However, since the Fourier transform of a quasi-crystal configuration consists of sharp delta peaks, we classify them as regular ground states, following the terminology in studies of dynamical systems [2, 3]. Another type is represented by ground states of the anti-ferromagnetic Ising model on a triangular lattice, which are often called disordered ones. The ground states are neither periodic nor quasi-periodic. However, since their entropy density is not zero as calculated explicitly [4], we do not regard such disordered ground states as irregularly ordered ground states. It is worthwhile noting that a string representation

§ sasa@jiro.c.u-tokyo.ac.jp

of the ground states is described by a stochastic rule corresponding to non-intersecting random walks [5, 6]. Based on these considerations, we define irregularly ordered ground states as those which have no delta peaks in their Fourier transform and whose entropy density is zero.

As an example with irregularly ordered ground states, one remembers the Frenkel-Kontorova model [7, 8], because its ground state is described by a chaotic map. Since it does not exhibit a phase transition at finite temperature, it is natural to consider an extended Frenkel-Kontorova model in two-dimensions. Recently, for such an extended model together with other related models, a certain type of transition has been found with the construction of ground states [9]. An interesting study with experimental relevance is now going on. However, from a theoretical viewpoint, the model is still complicated if one attempts to elucidate the nature of thermodynamic transitions associated with irregularly ordered ground states. In order to develop a theoretical argument, it seems better to study a two-dimensional lattice model. We here remark that non-trivial ground states in lattice gas models, which include an infinitely series of periodic ground states, were discussed in Refs. [10, 11]. Furthermore, we should mention that Ref. [12] reports a three-dimensional short-range interaction model in which non-periodic long-range order sustains at positive temperature. This reference also provides a summary of mathematical results on non-periodic order of ground states and Gibbs states for lattice models.

Based on these previous studies, in this paper, we first present a two-dimensional lattice gas model with irregularly ordered ground states. The ground states of our model are described by a one-dimensional cellular automaton whose deterministic rule yields a non-repetitive structure given by a superposition of Sierpinski gaskets. We next consider a possibility of thermodynamic transitions associated with the ground states. Since our model turns out to be self-dual for a duality transformation, we can present a simple argument for the thermodynamic transition.

2. Model

We consider hard-core particles in a triangle lattice consisting of N sites. Let Λ be the set of all sites in the lattice and Λ^* be the set of all upward triangles. We express a configuration of the particles by an occupation variable σ_i for $i \in \Lambda$: $\sigma_i = 1$ when site i is occupied by a particle, while $\sigma_i = 0$ when the site is empty. A particle configuration is collectively denoted by $\sigma = (\sigma_i)_{i \in \Lambda}$. For each upward triangle $j \in \Lambda^*$, we denote the sites at the top, left and right of the upward triangle by $t(j)$, $\ell(j)$, and $r(j)$, respectively. (See the left in figure 1.) We describe a soft interaction among particles in $j \in \Lambda^*$ by assuming a local energy V_j as follows: $V_j(\sigma) = 0$ when the particle number in j is zero or two, otherwise $V_j(\sigma) = J > 0$. Explicitly, one may write

$$V_j(\sigma) = J[(\sigma_{t(j)} + \sigma_{\ell(j)} + \sigma_{r(j)}) \bmod 2]. \quad (1)$$

Here, for a given site i , there are three upward triangles containing the site i . The upward triangles at the left, right and bottom of the site i are denoted by $\ell(i)$, $r(i)$,

and $b(i) \in \Lambda^*$, respectively. (See the center in figure (1).) We will see later that it is convenient to identify each upward triangle j with a dual site taken at the center of the same triangle. Then, the set Λ^* may be identified with the dual lattice, which also forms a triangular lattice. See the right in figure 1.

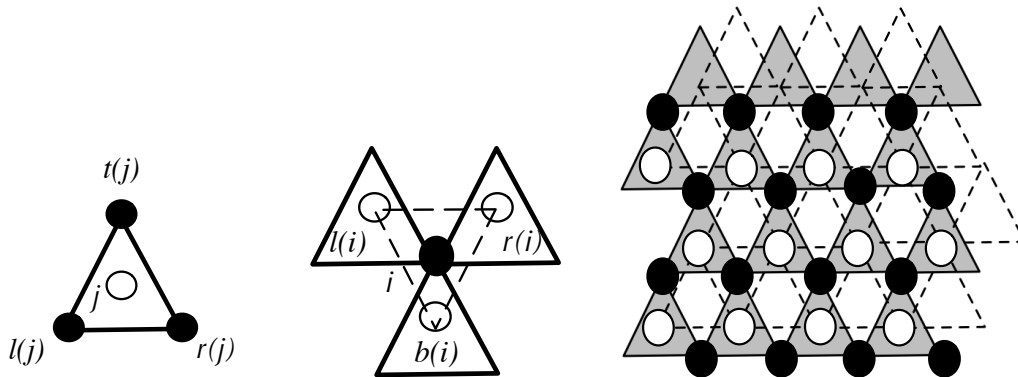


Figure 1. Filled circles represent sites in the original triangular lattice Λ , and empty circles represent sites in the dual lattice Λ^* .

We study the equilibrium statistical mechanics with the Hamiltonian $H(\sigma) = \sum_{j \in \Lambda^*} V_j(\sigma)$. When studying statistical mechanics, it is convenient to express

$$H(\sigma) = \frac{J}{2} \sum_{j \in \Lambda^*} [(2\sigma_{t(j)} - 1)(2\sigma_{\ell(j)} - 1)(2\sigma_{r(j)} - 1) + 1]. \quad (2)$$

All the thermodynamic properties of the system with temperature T and density ρ are described by the Helmholtz free energy density

$$f(T, \rho) = -T \lim_{N \rightarrow \infty} \frac{1}{N} \log Z(T, \rho). \quad (3)$$

Here, the partition function is given by

$$Z(T, \rho) = \sum_{\sigma} e^{-\beta H(\sigma)} \delta(N\rho, \sum_i \sigma_i), \quad (4)$$

where $\delta(\cdot, \cdot)$ is Kronecker's delta function. Throughout the paper, β is identical to $1/T$, and the Boltzmann constant is set to unity. When we report results of numerical experiments, we always assume $J = 1$. We also define the ground-state entropy explicitly as follows. Let $\Omega(E, \rho; N)$ be the number of particle configurations for a given density ρ and energy E . The entropy is defined by $S(E, \rho; N) = \log \Omega(E, \rho; N)$. By the ground-state entropy is meant $S_{\text{GS}}(\rho; N) = \min_E S(E, \rho; N)$, and its density $s_{\text{GS}}(\rho)$ is defined as $\lim_{N \rightarrow \infty} S_{\text{GS}}(\rho; N)/N$. Obviously, $s_{\text{GS}}(\rho) \geq 0$. Note that the free energy density $f(T, \rho)$ is related to the entropy as $f(T, \rho) = \lim_{N \rightarrow \infty} (E_* - TS(E_*, \rho; N))/N$, where E_* is determined by $\partial S(E, \rho)/\partial E|_{E=E_*} = \beta$.

The spin model equivalent to the Hamiltonian (2) was introduced by Newman and Moore [13] and studied further [14, 15]. (The equivalence is explicitly written in (8).)

These previous studies focused on the spin system without a magnetic field. As described later, this case corresponds to the lattice gas model with zero chemical potential or with half-filled density. A thermodynamic transition, which is our main concern, does not occur in this case.

Ground states: The ground states of the model are defined as configurations in the limit $T \rightarrow 0$. Since $H \geq 0$, the configurations satisfying $H(\sigma) = 0$ are ground-states. Obviously, $\sigma_i = 0$ for any i provides the ground state for the system with $\rho = 0$. As the other limiting case, the maximally packed ground states are easily found. They are crystals with $\rho = 2/3$. There are three configurations depending on its position.

The other ground states whose density is neither 0 nor $2/3$ are given by non-trivial configurations. In order to see them, let us consider the case that one particle is put on a site for the vacuum $\rho = 0$. Then, the energy is non-zero in the three upward triangles containing this site. Thus, one particle must be put in each upward triangle so as to minimize the energy. This iterative process is not repetition, but it is given by a simple rule.

We describe this rule explicitly. From the expression (1), one finds that the condition $V_j(\sigma) = 0$ is equivalent to the addition rule $\sigma_{t(j)} = \sigma_{\ell(j)} + \sigma_{r(j)} \pmod{2}$. Suppose that a particle configuration in the bottom line in the lattice is given. Then, when a particle configuration in the second bottom line is determined by applying the addition rule, the energy of upward triangles on the bottom line is zero. By repeating this process line by line, one obtains a particle configuration in Λ . This deterministic rule is equivalent to an elementary cellular automaton (CA) on a one-dimensional lattice. According to Wolfram's classification, it corresponds to Rule 102 included in class III [16], where space-time configurations generated by the rules in class III are known to be irregular for almost all initial conditions.

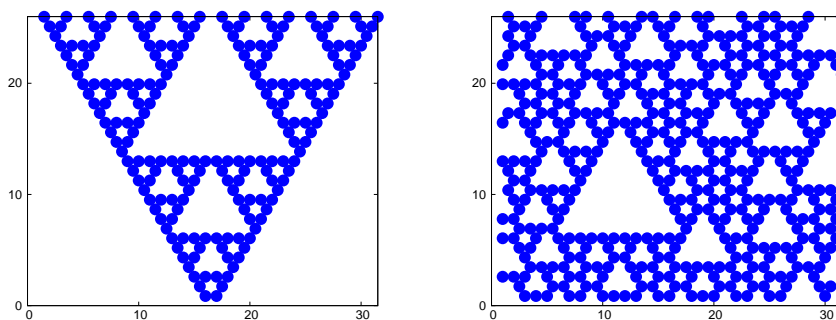


Figure 2. (Color online) Space-time configuration of the cellular automaton. The blue circles represent sites at which $\sigma_i = 1$. Periodic boundary conditions of the one-dimensional lattice (horizontal axis) are assumed, and time is the vertical axis. The initial conditions are given by a single seed at the center of the bottom line (left figure) and given randomly at the bottom line (right figure).

As the simplest example, in the left of figure 2, we display a configuration starting

from just one particle in the bottom line. It is called a Sierpinski gasket which is a famous fractal pattern with the fractal dimension $d_f = \log 3 / \log 2$. Since the rule is linear, the superposition of two configurations (in the module two) also satisfies the CA rule. Thus, all the configurations generated by the CA rule are obtained by superposition of Sierpinski gaskets. In the right of figure 2, we display a configuration starting from particles randomly placed on the bottom line.

Now, we consider the system with linear size L . That is, $N = L^2$. For simplicity, we first assume that the local energies for upward triangles whose bottom edge is at the top line or whose top site is at the bottom line are always zero. We also assume periodic boundary conditions at the side lines. With this choice of boundary conditions, all the particle configurations satisfying $H(\sigma) = 0$ are equivalent to space time configurations generated by L time steps evolution of the CA with the lattice size L . From the deterministic nature of the rule, the number of the configurations is 2^L . Therefore, the density of ground-state entropy is estimated as $s_{\text{GS}}(\rho) \leq \log 2 / L$ for any ρ , which leads to $s_{\text{GS}}(\rho) = 0$ in the thermodynamic limit.

For the other boundary conditions, to determine ground state configurations for a given ρ is not easy. Concretely, let us consider the system with periodic boundary conditions in all directions. In principle, zero-energy configurations for a given system size L can be determined by an algebraic method [17]. However, for example, it has been known that the number of the configurations depends on system size L in a quite complicated manner which comes from the arithmetic nature of L . Furthermore, in some values of L , say $L = 32$, there is no zero-energy configuration when $\rho \neq 0$. In this case, the ground state configuration involves defects, each of which is defined on an upward triangle with the energy J . The best positions of the defects for minimizing the energy would be determined in an irregular manner as a function of ρ and L . Although the precise argument in this case is quite difficult, we provide a rough estimation of a typical number of defects n_d as follows. We start with a simple observation that an isolated Sierpinski gasket with any size ℓ is generated by assuming a defect at each vertex of the largest triangle. The number of particles involved in the gasket is ℓ^{d_f} . Let n be the highest level of the gasket included in the system. Then, $2^n \simeq O(L)$. When the particle density is finite, the number of gaskets is $O(L^{2-d_f})$. Since there are three defects in each gasket, $n_d \simeq O(L^{2-d_f})$. Therefore, the ground-state energy is $O(L^{2-d_f})$ and the density of ground-state entropy is estimated as $s_{\text{GS}} \simeq O(\log 2 / L) + O(n_d / N) \simeq O(L^{-1}) + O(L^{-d_f})$, which leads to $s_{\text{GS}}(\rho) = 0$ in the thermodynamic limit.

3. Statistical mechanics

Following a standard method in statistical mechanics, we consider the grand partition function

$$\Xi(T, \mu) = \sum_{\sigma} e^{-\beta[H(\sigma) - \mu \sum_i \sigma_i]}. \quad (5)$$

The pressure $p(T, \mu)$ in the model is given by

$$p(T, \mu) = T \lim_{N \rightarrow \infty} \frac{1}{N} \log \Xi(T, \mu), \quad (6)$$

and the free energy density $f(T, \rho)$ is obtained by the Legendre transformation

$$f(T, \rho) = \sup_{\mu} [\mu \rho - p(T, \mu)]. \quad (7)$$

Furthermore, by introducing a spin variable $s_i \equiv 2\sigma_i - 1$ and parameters $K_1 = \beta J/2$ and $K_2 = -\beta \mu/2$, we express $\Xi(T, \mu) = e^{-(K_1 + K_2)N} Y(K_1, K_2)$ as

$$Y(K_1, K_2) = \sum_s e^{-K_1 \sum_{j \in \Lambda^*} s_{t(j)} s_{\ell(j)} s_{r(j)} - K_2 \sum_{i \in \Lambda} s_i}, \quad (8)$$

where $s = (s_i)_{i \in \Lambda}$. The partition function Y is equivalent to that for the three-body Ising model on upward triangles under a magnetic field. Note that the case $K_2 = 0$ was studied in Refs. [13, 14, 15] and that the three-body Ising model on all triangles without a magnetic field was solved exactly [18].

We start our analysis from the easiest case $K_1 \gg 1$ and $K_2 \simeq O(1)$, under which configurations minimizing $\sum_{j \in \Lambda^*} s_{t(j)} s_{\ell(j)} s_{r(j)}$ contribute to Y . We assume boundary conditions such that all the spins outside the system are down. Then, the minimizer is uniquely determined as $s_i = -1$ for all i . We thus obtain

$$Y(K_1, K_2) \simeq \exp((K_1 + K_2)N) \quad (9)$$

as the leading order contribution. This result leads to $p(T, \mu) \simeq 0$. The first order correction to (9) arises from a single spin-flip with the probability $\exp(-3\beta J)$. This means

$$p(T, \mu) = O(e^{-3\beta J}). \quad (10)$$

Duality relation: Next we derive a duality relation for $p(T, \mu)$, which is presented in (23). In the argument below, we assume $K_2 \geq 0$. By making a change of variable $s_i \rightarrow -s_i$ in the sum of (8), we have a relation

$$Y(K_1, K_2) = Y(-K_1, -K_2). \quad (11)$$

With this relation, the expansion of the exponential function yields

$$Y(K_1, K_2) = C \sum_s \left[\prod_{j \in \Lambda^*} (1 + s_{t(j)} s_{\ell(j)} s_{r(j)} \tanh K_1) \right] \left[\prod_{i \in \Lambda} (1 + s_i \tanh K_2) \right], \quad (12)$$

where $C = (\cosh K_1)^N (\cosh K_2)^N$. We then introduce a new variable $\tilde{\sigma}_j$ whose value is either 0 or 1 for $j \in \Lambda^*$. Concretely, $\tilde{\sigma}_j = 1$ when the term $s_{t(j)} s_{\ell(j)} s_{r(j)} \tanh K_1$ is picked up in the expansion of the first product. Otherwise, $\tilde{\sigma}_j = 0$. In terms of this new variable, the first product is rewritten as

$$\begin{aligned} \prod_{j \in \Lambda^*} (1 + s_{t(j)} s_{\ell(j)} s_{r(j)} \tanh K_1) &= \sum_{\tilde{\sigma}} \prod_{j \in \Lambda^*} (s_{t(j)} s_{\ell(j)} s_{r(j)} \tanh K_1)^{\tilde{\sigma}_j} \\ &= \sum_{\tilde{\sigma}} (\tanh K_1)^{\sum_{j \in \Lambda^*} \tilde{\sigma}_j} \prod_{i \in \Lambda} s_i^{\tilde{\sigma}_{\ell(i)} + \tilde{\sigma}_{r(i)} + \tilde{\sigma}_{b(i)}}, \end{aligned} \quad (13)$$

where $\tilde{\sigma} = (\tilde{\sigma}_j)_{j \in \Lambda^*}$ and we have rearranged the product as that over $i \in \Lambda$. Note that $\ell(i)$, $r(i)$, and $b(i)$ were defined previously. See figure 1. By substituting this expression into (12), we obtain

$$Y(K_1, K_2) = C \sum_s \sum_{\tilde{\sigma}} (\tanh K_1)^{\sum_{j \in \Lambda^*} \tilde{\sigma}_j} \left[\prod_{i \in \Lambda} (s_i^{\tilde{\sigma}_{\ell(i)} + \tilde{\sigma}_{r(i)} + \tilde{\sigma}_{b(i)}} + \tanh K_2 s_i^{\tilde{\sigma}_{\ell(i)} + \tilde{\sigma}_{r(i)} + \tilde{\sigma}_{b(i)} + 1}) \right]. \quad (14)$$

Here, we define K_1^* by

$$\exp(-2K_1^*) = \tanh K_2, \quad (15)$$

and introduce a variable $\tilde{s}_j = 2\tilde{\sigma}_j - 1$. By an explicit calculation, we can confirm

$$\sum_{s_i} (s_i^{\tilde{\sigma}_{\ell(i)} + \tilde{\sigma}_{r(i)} + \tilde{\sigma}_{b(i)}} + \tanh K_2 s_i^{\tilde{\sigma}_{\ell(i)} + \tilde{\sigma}_{r(i)} + \tilde{\sigma}_{b(i)} + 1}) = 2e^{-K_1^*(\tilde{s}_{\ell(i)}\tilde{s}_{r(i)}\tilde{s}_{b(i)} + 1)}. \quad (16)$$

Similarly, we write

$$(\tanh K_1)^{\sum_{j \in \Lambda^*} \tilde{\sigma}_j} = e^{-K_2^* \sum_{j \in \Lambda^*} (\tilde{s}_j + 1)}, \quad (17)$$

where K_2^* has been defined by

$$\exp(-2K_2^*) = \tanh K_1. \quad (18)$$

By substituting (16) and (17) into (14), we obtain

$$Y(K_1, K_2) = 2^N C e^{-K_2^* N^*} e^{-K_1^* N^*} \sum_{\tilde{s}} e^{-K_2^* \sum_{j \in \Lambda^*} \tilde{s}_j} e^{-K_1^* \sum_{i \in \Lambda} \tilde{s}_{\ell(i)} \tilde{s}_{r(i)} \tilde{s}_{b(i)}}, \quad (19)$$

where $\tilde{s} = (\tilde{s}_j)_{j \in \Lambda^*}$ and N^* is the number of elements in Λ^* . We have $N^* = N$ when we assume periodic boundary conditions. By recalling that Λ^* may be identified with the dual lattice, and by comparing (19) with (8), one finds that the sum in (19) is nothing but the partition function of the same model with the new coupling constants K_1^* and K_2^* defined on the dual lattice Λ^* . See figure 1 again. The only and irrelevant difference is that the particles now interact with each other on downward triangles. We thus find the duality relation

$$Y(K_1, K_2) = 2^N (\cosh K_1)^N (\cosh K_2)^N e^{-(K_1^* + K_2^*)N} Y(K_1^*, K_2^*). \quad (20)$$

We further simplify (15), (18), and (20) as

$$Y(K_1, K_2) = Y(K_1^*, K_2^*) (\sinh 2K_1 \sinh 2K_2)^{N/2}, \quad (21)$$

and

$$(\sinh 2K_1^*) (\sinh 2K_2) = (\sinh 2K_2^*) (\sinh 2K_1) = 1. \quad (22)$$

Finally, we define $T^* = 1/\beta^*$ and μ^* by $K_1^* = \beta^* J/2$ and $K_2^* = -\beta^* \mu^*/2$. Then, (21) yields

$$p(T, \mu) = p(T^*, \mu^*) - \frac{J}{2} + \frac{\mu}{2} + T \log \left(2 \cosh \frac{J}{2T} \cosh \frac{\mu}{2T} \right). \quad (23)$$

Note that a duality relation connecting large β to small $\beta\mu$ was discussed in Ref. [19].

Exact result for $\rho = 0.5$: As an application of the duality relation (23), we calculate the free energy density $f(T, \rho = 0.5)$ exactly. When $|\mu| \ll 1$, the dual point $T^* \ll 1$ satisfies $\exp(-J/T^*) \simeq -2\mu/T$ for any T . Since the pressure $p(T^*, \mu^*)$ in the regime $T^* \ll 1$ is known as (10), we substitute it into (23). Noting that $O(e^{-3\beta^*J}) = O(|\mu|^3)$, we derive

$$p(T, \mu) = -\frac{J}{2} + \frac{\mu}{2} + T \left[\log \left(2 \cosh \frac{J}{2T} \right) + O(|\mu|^2) \right] \quad (24)$$

for $|\mu| \ll 1$. Since

$$\rho = \left. \frac{\partial p(T, \mu)}{\partial \mu} \right|_{\mu=0} = \frac{1}{2}, \quad (25)$$

we obtain from (7)

$$f(T, \rho = 0.5) = \frac{J}{2} - T \left[\log \left(2 \cosh \frac{J}{2T} \right) \right]. \quad (26)$$

This free energy density is equivalent to that of non-interacting Ising spins. Essentially the same result was obtained in Ref. [13]. Here, recall that the ground state of the system with $\rho = 0.5$ is given by superposition of the Sierpinski gaskets. Therefore, in contrast to the simple form of the free energy density, equilibrium configurations are complex as displayed in the left of figure 3. We then note that the equilibration time is extremely large, which might originate from complex configurations in the system with large β . In the right of figure 3, we plot the heat capacity obtained numerically with the aid of an exchange Monte Carlo method [20]. The results for $\beta \geq 4$ still depend on the waiting time within our observations. This means that equilibrium states are not produced yet when $\beta \geq 4$. Indeed, the numerical data for $\beta \geq 4$ are different from the theoretical curve derived exactly. One may interpret that the system is in a dynamical glass phase. See Refs. [13, 14, 15] for detailed studies of dynamical properties in this regime of the model. With regard to this problem, we also remark that the mean-field model of the ferro-magnetic three-body Ising model without a magnetic field exhibits a glass transition in a meta-stable branch as well as a thermodynamic transition to a ferro-magnetic phase [21].

Thermodynamic transition: The most standard application of duality relations is to provide candidates of thermodynamically singular points. Indeed, if $p(T, \mu)$ is singular at some point (T_0, μ_0) , $p(T, \mu)$ is singular at (T_0^*, μ_0^*) too. Thus, a thermodynamic transition occurs on the self-dual line

$$(\sinh J/T)(\sinh \mu/T) = -1 \quad (27)$$

if there is one transition point in $0 < T < \infty$ for fixed $\mu < 0$. Note that, in general, there is no reason to assume the latter condition, although there are many successful examples since the pioneering paper [22]. As one example, let us consider the case where $T \gg 1$. Then, the self-dual point is evaluated as $\mu \simeq -T \log T$. It is hardly expected that a transition occurs in such a high-temperature and largely negative chemical potential

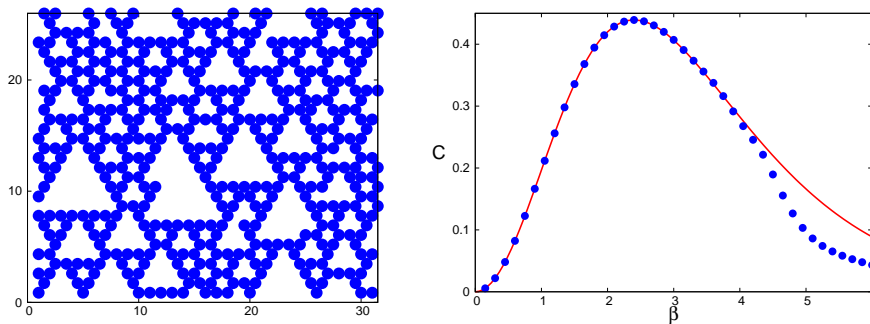


Figure 3. (Color online) Numerical experiment of the model with $\mu = 0$. $N = 1024$. The left figure shows an equilibrium configuration for $\beta = 3.75$. The blue circles represent particles. The right graph is the heat capacity C as a function β . The circle symbols represent experimental results, where the data for $\beta \geq 4$ still depend on a waiting time within our observation. The solid line is the exact result derived theoretically.

regime. Thus, without a hasty conclusion, it is necessary to check whether or not transitions occur on the self-dual line.

As another tractable case, we consider the system with $0 < -\mu/T \ll 1$ fixed. For sufficiently small T , we have $p(T, \mu) \simeq 0$ as derived in (10). In this case, $\rho \simeq 0$. Now, we increase T from the region $p(T, \mu) \simeq 0$ (with keeping $T \ll 1$) and investigate the instability of the state $\rho \simeq 0$. Following a standard phenomenological argument [23], we replace a macroscopic spherical domain by a spherical domain whose pressure is given by (24). The pressure difference from the bulk region is estimated by

$$\Delta p \simeq \frac{\mu}{2} + T \exp(-J/T), \quad (28)$$

where we have used (24). If $\Delta p > 0$, the inserted domain grows if surface effects are ignored. That is, the first-order transition occurs at $\Delta p = 0$, which leads to

$$\frac{\mu}{2T} \exp(J/T) = -1. \quad (29)$$

The equality coincides with the leading order equation of (27) under an asymptotic condition that $0 < -\mu/T \ll 1$ and $T \ll 1$. Therefore, we expect that the self-dual line under this condition provides actual transition points.

In figure 4, we display a result of numerical experiments for the system with $\mu = -0.04$ fixed. It is seen that the density exhibits the discontinuous change from $\rho_1(\mu)$ to $\rho_2(\mu)$ at $\beta = \beta_{\text{dis}}(\mu)$, where the left of figure 4 shows that $2.75 < \beta_{\text{dis}} < 3.0$. Since the dual relation (27) gives $\beta_{\text{dis}} \simeq 2.86$ for $\mu = -0.04$, we judge that the theoretical consideration is consistent with the result of the numerical experiment. An equilibrium configuration in the lower temperature phase ($T < T_{\text{dis}}(\mu)$) is almost vacuum, while it is superposition of Sierpinski gaskets in the higher temperature phase ($T_{\text{dis}}(\mu) < T \ll 1$). Interestingly, as shown in figure 5, the intensity of density fluctuations $\chi = N \langle (\rho - \langle \rho \rangle)^2 \rangle$ measured with (T, μ) fixed exhibits a power-law behavior $\chi \simeq (\beta_{\text{dis}} - \beta)^{-1/2}$ in the higher temperature side, while no divergent behavior in the lower temperature side. Similar

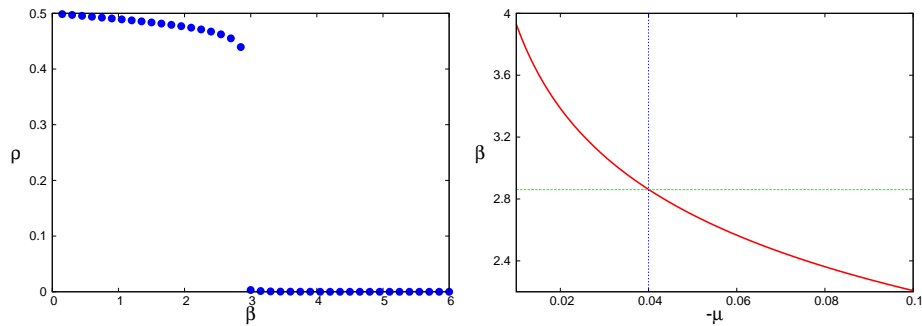


Figure 4. (Color online) (Left): ρ versus β obtained by numerical experiments of the model with $\mu = -0.04$. $N = 1024$. (Right): The self-dual relation given by (27). Note that $\beta = 2.86$ when $\mu = -0.04$.

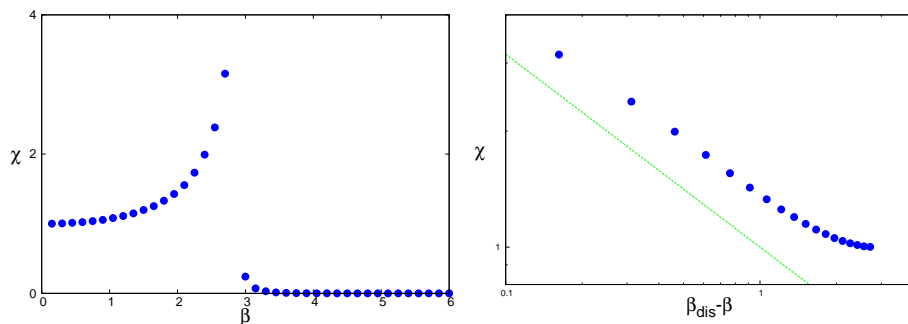


Figure 5. (Color online) (Left): χ versus β obtained by numerical experiments of the model with $\mu = -0.04$. $N = 1024$. (Right): Log-log plot of χ as a function of $\beta_{\text{dis}} - \beta$ for $\beta < \beta_{\text{dis}}$. The guide line represents $\chi = (\beta_{\text{dis}} - \beta)^{-1/2}$.

behavior was observed in several models [5]. Furthermore, we note that the transition temperature $T_{\text{dis}}(\mu)$ approaches zero as $\mu \rightarrow 0$. The equilibration becomes very hard as $|\mu|$ is decreased. Indeed, we did not observe the first-order transition for the system with $\mu = -0.02$ for $N = 1024$ within our observation time. In the left of figure 6, we present a schematic phase diagram in the (μ, T) space, where $\mu \leq 0$. Since there is no phase transition for sufficiently large T , the first-order transition line in the state space possesses a terminal point (μ_s, T_s) .

Let us consider a schematic phase diagram in the state space (ρ, T) . Since there exists a crystal configuration, a transition to a crystal state is expected to occur in the dense regime with $\rho > 0.5$. Indeed, we observed it by a preliminary numerical experiment. However, in this paper, we restrict our investigation to the regime $\rho \leq 0.5$ in order to present a clear argument.

We first recall that the density changes discontinuously from $\rho_1(\mu)$ to $\rho_2(\mu)$ at $T_{\text{dis}}(\mu)$ in decreasing the temperature with $\mu_s < \mu < 0$ fixed. See the dotted line in the right of figure 6. Then, the region below the two curves $(\rho_1(\mu), T_{\text{dis}}(\mu))$ and $(\rho_2(\mu), T_{\text{dis}}(\mu))$, with $\mu_s \leq \mu \leq 0$, is a coexistence phase that corresponds to the transition line in the left of figure 6.

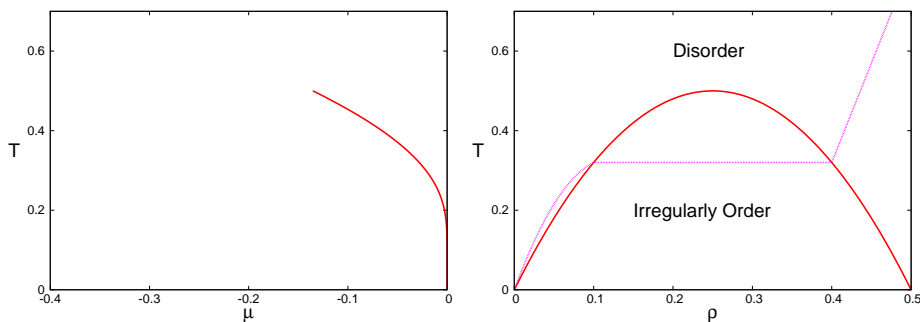


Figure 6. (Color online) Schematic phase diagrams in the state space (μ, T) (left) and in the state space (ρ, T) (right). In order to see the qualitative behavior more easily, the graphs are not accurately displayed. The chemical potential is equal to along the dotted line in the right figure. The coexistence phase is labeled by “Irregularly Order”, but its non-trivial nature is not fully explored yet. See a discussion in the text.

Now, we fix ρ satisfying $0 < \rho < 1/2$. There exists a special temperature $T_c(\rho)$ below which the system is in the coexistence phase. Note that $d\mu/d\rho|_T = 0$ holds in this phase. We further fix T to be smaller than $T_c(\rho)$. The chemical potential μ for a given (T, ρ) is determined uniquely. Then, from the analogy with a liquid-gas transition, one may imagine that two phases, $(T, \rho_1(\mu))$ and $(T, \rho_2(\mu))$, are separated. Note that $\rho_1 \simeq 0$ and $\rho_2 \simeq 1/2$ when T is sufficiently small (that is, μ is sufficiently close to 0). Here, if this picture is correct, the interfacial energy proportional to $O(L)$ remains in the limit $T \rightarrow 0$. However, as discussed in section 2, the ground states are far from such simple configurations. At the end of section 2, we conjectured that point defects appear with the energy $O(L^{2-d_f})$ in general ground states. Since this is less than the interfacial energy $O(L)$, we expect that phase separated configurations are not realized in the ground states.

Of course, even if phase separated configurations do not appear in the ground states, this does not ensure the non-trivial nature of the system with finite temperature. We need to investigate the finite temperature system directly. More explicitly, we conjecture that the number of pure states in the coexistence phase is not two, but continuously distributed with a parameterization of density. That is, for example, when observing a density just on the first-order transition point in the (T, μ) ensemble, its distribution function may form a continuous function, not a two-peaks function, in the thermodynamic limit. To prove this conjecture mathematically is a challenging problem, but careful numerical investigations will be done in future. With expecting the validity of our conjecture, we call the coexistence phase *irregularly ordered phase*.

4. Future problems

Before ending this paper, we list up problems to be studied in future. First of all, a precise phase diagram should be determined. In order to complete it, we will study the behavior near the critical point and the transition lines in detail. After the determination

of the phase boundaries, we will characterize each phase. Among the phases, the most non-trivial is the irregularly ordered phase. As an example, in figure 7, we present configurations for $\rho = 0.25$. The case $\beta = 3.0$ (left) is in the disordered phase, while the case $\beta = 4.5$ (right) is in the irregularly ordered phase. Both the configurations were obtained by long-time calculation of an exchange Monte Carlo method. The waiting time dependence is relatively small, but more careful checks are necessary to judge whether the system reaches the equilibrium state in the irregularly ordered phase. Numerical studies on this phase are quite challenging.

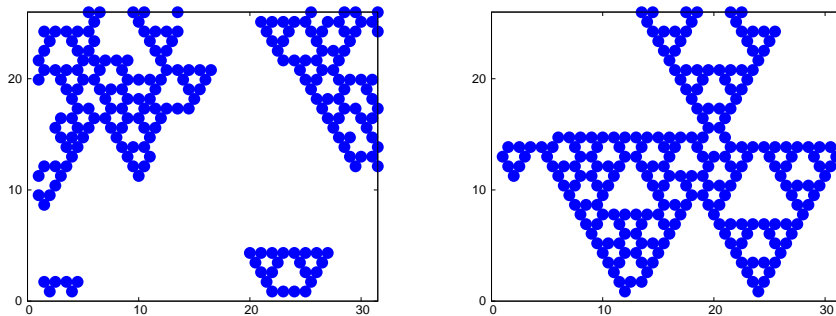


Figure 7. (Color online) Configurations for the system with $\rho = 0.25$ fixed. The blue circles represent particles. $\beta = 3.0$ (Left) and $\beta = 4.5$ (Right)

Theoretically, the next step study is to construct a perturbation theory for the system with small T and small $|\mu|$ in order to understand peculiar features observed numerically. This study will formulate calculation techniques for treating excitations of fractal patterns. Here let us recall that the mapping to a free gas of defects was useful to understand behaviors for the system with $\mu = 0$ [14, 15]. It is then a natural idea to describe the small $|\mu|$ system through a weak interaction among defects. For example, it might be interesting if one confirms that defects form a bounded state in the irregularly ordered state. Furthermore, the study on algebraic properties of the cellular automaton rule may provide a hint for characterizing the irregularly ordered phase. As a different direction of study, one may investigate the irregularly ordered phase from a viewpoint of thermodynamic glass. At present, the existence of thermodynamic glass in finite dimensions is not established yet, mainly because dynamical singularities cover the equilibrium nature. Nevertheless, the understanding at the mean-field level has been greatly accumulated. In particular, there is consensus that thermodynamic glasses at the mean-field level are characterized by a one-step replica-symmetry breaking [24, 25]. Recently, a thermodynamic glass phase in a lattice model [26] has been investigated numerically along with this idea [27]. As did in the study, one might argue a replica-symmetry breaking in the irregularly ordered phase of our model.

Finally, we remark that our model has no direct correspondence with experimental systems. However, needless to say, it is quite amazing to find phase transitions associated with irregularly ordered ground states in natural phenomena. (See Ref. [28] for some connection of the model to experimental systems.) We expect that the phenomenon

reported in this paper will be studied further theoretically and experimentally.

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References

- [1] Janssen T 1988 Physics Report **168** 55
- [2] Powell G E and Percival I C 1979 J. Phys. A: Math. Gen, **12** 2053
- [3] Eckmann J P and Ruelle D 1985 Rev. Mod. Phys. **57** 617
- [4] Wannier G H 1950 Phys. Rev. **79** 357
- [5] Blöte H W J and Hilhorst H J, 1982 J. Phys. A: Math. Gen. **15** L 631
- [6] Dhar A, Chaudhuri P and Dasgupta C 2000 Phys. Rev. B **61** 6227
- [7] Aubry S and Le Daeron P Y 1983 Physica D **8** 381
- [8] Peyrard M and Aubry S 1983 J. Phys. C: Solid State Phys **16** 1593
- [9] Yoshino H, Nogawa T and Kim B 2010 arXiv:1004.0585
- [10] Kanamori J 1984 J. Phys. Soc. Jpn. **53** 250
- [11] Dublennykh Y I 2009 Phys. Rev. E **80** 011123
- [12] van Enter A C D, Miekisz K, and Zahradnik M 1998 J. Stat. Phys. **90** 1441
- [13] Newman M E J and Moore C 1999 Phys. Rev. E **60** 5068
- [14] Garrahan J P and Newman M E J 2000 Phys. Rev. E **62** 7670
- [15] Jack R and Garrahan J P 2005 J. Chem. Phys **123** 164508
- [16] Wolfram S 1983 Rev. Mod. Phys. **55** 601
- [17] Martin O, Odlyzko A M and Wolfram S 1984 Commun. Math. Phys. **93** 219
- [18] Baxter R J 2007 *Exactly solved models in statistical mechanics* (Dover, New York)
- [19] Balian R, Drouffe J M and Itzykson C 1975 Phys. Rev. D **11** 2098
- [20] Hukushima K and Nemoto K 1996 J. Phys. Soc. Jpn. **65** 1604
- [21] Franz S, Mezard M, Ricci-Tersenghi F, Weigt M and Zecchina 2001 Europhys. Lett. **55** 465
- [22] Kramers H A and Wannier G H 1941 Phys. Rev. **60** 252
- [23] L. D. Landau and E. M. Lifshitz, *Statistical Physics, 3rd ed.*, (Pergamon Press, Oxford, 1990).
- [24] Parisi G and Zamponi F 2010 Rev. Mod. Phys. **82** 789
- [25] Mezard M and Parisi G 2009 arXiv:0910.2838
- [26] Pica Ciamarra M, Tarzia M, de Candia A, and Coniglio A 2003 Phys. Rev. E. **67** 057105
- [27] Parisi G 2009 arXiv:0911.2265
- [28] Barkema G T, Newman M E J and Breeman M 1994 Phys. Rev. B **50** 7946